

SAFETY DATA SHEET

Creation Date 25-Jan-2011

Revision Date 24-Dec-2021

Revision Number 5

1. Identification

Product Name 1-Hexanethiol

Cat No. : AC215270000; AC215270050; AC215271000; AC215275000

CAS No 111-31-9
Synonyms Hexyl mercaptan

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number For information **US** call: 001-800-ACROS-01 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No.**US**:001-800-424-9300 / **Europe**:001-703-527-3887

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids	Category 3
Acute oral toxicity	Category 4
Acute Inhalation Toxicity - Vapors	Category 3

Label Elements

Signal Word

Danger

Hazard Statements

Flammable liquid and vapor
Harmful if swallowed
Toxic if inhaled

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Avoid breathing dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area
Keep away from heat/sparks/open flames/hot surfaces. - No smoking
Keep container tightly closed
Ground/bond container and receiving equipment
Use explosion-proof electrical/ventilating/lighting equipment
Use only non-sparking tools
Take precautionary measures against static discharge
Wear protective gloves/protective clothing/eye protection/face protection
Keep cool

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
Call a POISON CENTER or doctor/physician

Skin

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower

Ingestion

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
Rinse mouth

Fire

In case of fire: Use CO₂, dry chemical, or foam for extinction

Storage

Store in a well-ventilated place. Keep container tightly closed
Store locked up

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

Other hazards

Stench.

3. Composition/Information on Ingredients

Component	CAS No	Weight %
1-Hexanethiol	111-31-9	>95

4. First-aid measures

General Advice

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

Eye Contact

In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

Skin Contact

Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes.

Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.
Ingestion	Do NOT induce vomiting. Call a physician or poison control center immediately.
Most important symptoms and effects	. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Carbon dioxide (CO ₂). Dry chemical. Water mist may be used to cool closed containers. Chemical foam. Water mist may be used to cool closed containers.
Unsuitable Extinguishing Media	No information available
Flash Point	30 °C / 86 °F
Method -	No information available
Autoignition Temperature	No information available
Explosion Limits	
Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Flammable. Vapors may travel to source of ignition and flash back. Containers may explode when heated. Vapors may form explosive mixtures with air.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂). Sulfur oxides. Sulfides.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

NFPA

Health	Flammability	Instability	Physical hazards
3	2	0	N/A

6. Accidental release measures

Personal Precautions	Ensure adequate ventilation. Use personal protective equipment as required. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas. Remove all sources of ignition. Take precautionary measures against static discharges.
Environmental Precautions	Should not be released into the environment.
Methods for Containment and Clean Up	Keep in suitable, closed containers for disposal. Soak up with inert absorbent material. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

7. Handling and storage

Handling	Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Take
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precautionary measures against static discharges.

Storage.

Keep away from heat, sparks and flame. Flammables area. Keep container tightly closed in a dry and well-ventilated place. Incompatible Materials. Bases. Strong oxidizing agents. Metals. Reducing Agent.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH IDLH	Mexico OEL (TWA)
1-Hexanethiol			Ceiling: 0.5 ppm Ceiling: 2.7 mg/m ³	

Legend

NIOSH IDLH: NIOSH - National Institute for Occupational Safety and Health

Engineering Measures

Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting equipment.

Personal Protective Equipment**Eye/face Protection**

Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection

Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Colorless
Odor	Stench
Odor Threshold	No information available
pH	No information available
Melting Point/Range	-81 - -80 °C / -113.8 - -112 °F
Boiling Point/Range	150 - 154 °C / 302 - 309.2 °F @ 760 mmHg
Flash Point	30 °C / 86 °F
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	> 3.0
Specific Gravity	0.840
Solubility	Insoluble in water
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	400 °C
Viscosity	No information available
Molecular Formula	C6 H14 S
Molecular Weight	118.24

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions.
Conditions to Avoid	Keep away from open flames, hot surfaces and sources of ignition. Exposure to air. Incompatible products.
Incompatible Materials	Bases, Strong oxidizing agents, Metals, Reducing Agent
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO ₂), Sulfur oxides, Sulfides
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
1-Hexanethiol	LD50 = 1254 mg/kg (Rat)	Not listed	LC50 = 1080 ppm (Rat) 4 h

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation	No information available
Sensitization	No information available
Carcinogenicity	The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
1-Hexanethiol	111-31-9	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure None known

STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects, both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

Endocrine Disruptor Information No information available

Other Adverse Effects The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

Do not empty into drains. .

Persistence and Degradability Insoluble in water Persistence is unlikely based on information available.**Bioaccumulation/ Accumulation** No information available.**Mobility** Is not likely mobile in the environment due its low water solubility. Will likely be mobile in the environment due to its volatility.

Component	log Pow
1-Hexanethiol	5.35

13. Disposal considerations**Waste Disposal Methods** Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.**14. Transport information****DOT**

UN-No UN3071
 Proper Shipping Name Mercaptans, liquid, toxic, flammable, n.o.s.
 Hazard Class 6.1
 Subsidiary Hazard Class 3
 Packing Group II

TDG

UN-No UN3071
 Proper Shipping Name Mercaptan mixture, liquid, toxic, flammable, n.o.s.
 Hazard Class 6.1
 Subsidiary Hazard Class 3
 Packing Group II

IATA

UN-No UN3071
 Proper Shipping Name Mercaptan mixture, liquid, toxic, flammable, n.o.s.
 Hazard Class 6.1
 Subsidiary Hazard Class 3
 Packing Group II

IMDG/IMO

UN-No UN3071
 Proper Shipping Name Mercaptans, liquid, toxic, flammable, n.o.s.
 Hazard Class 6.1
 Subsidiary Hazard Class 3
 Packing Group II

15. Regulatory information**United States of America Inventory**

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
1-Hexanethiol	111-31-9	X	ACTIVE	-

Legend:**TSCA** - US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

- - Not Listed

TSCA 12(b) - Notices of Export Not applicable

International Inventories

Canada (DSL/NDL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
1-Hexanethiol	111-31-9	X	-	203-857-0	X	X	X	X	X	KE-19793

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

U.S. Federal Regulations

SARA 313	Not applicable
SARA 311/312 Hazard Categories	See section 2 for more information
CWA (Clean Water Act)	Not applicable
Clean Air Act	Not applicable
OSHA - Occupational Safety and Health Administration	Not applicable
CERCLA	Not applicable

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
1-Hexanethiol	-	X	-	-	-

U.S. Department of Transportation

Reportable Quantity (RQ):	N
DOT Marine Pollutant	N
DOT Severe Marine Pollutant	N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

Authorisation/Restrictions according to EU REACH**Safety, health and environmental regulations/legislation specific for the substance or mixture**

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
1-Hexanethiol	111-31-9	Not applicable	Not applicable	Not applicable	Not applicable

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)

1-Hexanethiol	111-31-9	Not applicable	Not applicable	Not applicable	Not applicable
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16. Other information

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Revision Summary This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS